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Calculation of Electrical Resistivity of Dislocations and Grain Boundaries in Polyvalent and Transition Metals

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Abstract – A dislocation model that takes into account the presence of quasistationary states and the lattice dilatation in the region of a dislocation core is used to perform a calculation concerning the electrical resistivity of polyvalent and transition metals from dislocations and grain boundaries. A low-angle grain boundary is treated as a set of dislocations, while a high-angle grain boundary is considered as a set of cylindrical pores. When the dilatation was assumed to be $dV = b_B^2$ (b_B is the stable Burgers vector of a perfect dislocation), a satisfactory agreement with the experimental data was obtained.

INTRODUCTION

Dislocations and grain boundaries are the most widespread defects in metals and determine their strength characteristics and performance. The problem of high electrical resistivity of dislocations and grain boundaries was first considered several decades ago, but as yet no satisfactory explanation of this phenomenon exists. Initial calculations of the grain boundary (ρ_G) [1, 2] and dislocation (ρ_d) [3, 4] contributions to electrical resistivity gave values of one or two orders of magnitude lower than those observed experimentally. Harrison [5], who took into account the lattice dilatation during plastic deformation and the fact that this dilatation was confined primarily within the region of the dislocation cores, was the first to obtain the correct order of magnitude for ρ_d. However, this model explained neither the magnitude nor the sign of the effect of dislocations on thermal emf [6]. Further progress in studying the effects of dislocations on transport properties was made when quasistationary electronic states were taken into account [7, 8], the existence of which was theoretically predicted [9] and then confirmed experimentally [10]. The resonance scattering of conduction electrons at these quasistationary states, lying near the Fermi level, gave values of ρ_d close to the experimental ones for a number of metals [7]; the best agreement was obtained in the case of nontransition metals. In [11] a grain boundary was treated as a set of resonantly scattering dislocations. The grain boundary contribution to electrical resistivity, calculated within such a model, was shown to be of the same order of magnitude as observed experimentally in nontransition metals. However, this model, used in [7, 9, 11], was criticized for uncertainty in the nature of perturbations leading to the appearance of resonances; in addition, the resistivities, calculated within this model, appear to be independent of the type of dislocation and the magnitude of its Burgers vector [12, 13]. As to the calculations of ρ_G in [11], we note that only the low-angle grain boundaries with misorientation angle $\theta < 15°$ can be described by a set of dislocations. In addition, the calculations of [11] were carried out for the particular case of columnar grains in thin films, and thus the distance between dislocations, composing the grain boundary, was two to three times smaller than in bulk samples; being perpendicular to the current, such dislocations gave the maximum contribution to electrical resistivity.

A recent paper [13] proposed that the Bragg scattering of conduction electrons at the boundaries of the Brillouin zone caused the high electrical resistivity of dislocations in metals. With only one adjustable parameter, numerical calculations for sixteen metals satisfactorily agreed with experimental results.

References [6, 14] explain the contributions of dislocations and grain boundaries to electrical resistivity and thermal emf of monovalent metals (Cu, Ag, Au) within a combined model that takes into account both the presence of resonance quasistationary states and the known experimental data on the structure of dislocation core (namely, the lattice dilatation and excess negative charge caused by this dilatation). We use this approach to calculate the electrical resistivity of dislocations and grain boundaries in more complex polyvalent and transition metals. Because the potential used in this study differs from that used in [6, 14], we present our calculations for copper and gold for the sake of completeness.

PRELIMINARY NOTES

The nearly complete occupation of the first Brillouin zone and its small overlapping with the second zone is the distinguishing feature of the electronic structure in the divalent metals. For this reason, the concentration of charge carriers in these metals is very small, and at present it can be evaluated from the band structure calculations only. The transport properties of transition metals (including ferromagnetic metals) are the phenomena most complex and difficult to explain, because these metals have two partially filled overlapping bands (*s* and *d*) near the Fermi level, and the *d*-band consists of two subbands with different spin orientations and different occupancies. The earlier theory of Mott [15] is the most suitable for describing the electronic properties of transition metals. According to this theory, because of the narrowness of the *d*-band and the high degree of its occupancy, the density of states N_d and the effective mass of charge carriers (holes) m_p^* in transition metals are considerably higher in the *d*-band as compared with the *s*-band, that is $N_d \gg N_s$ and $m_p^* > m_e^*$. The holes essentially do not contribute to the transport phenomena, but they are effective scattering centers for the *s*-electrons, because of the high probability of *s*–*d* transitions. It is assumed that the number of electrons of spin up (↑) in the *s*-band is equal to the number of *s*-electrons of spin down (↓), and the scattering of *s*-electrons to free *s*- and *d*-states is not accompanied by flip. Such an assumption is valid in the lowest order of the perturbation theory if one neglects spin-orbit coupling.

The Mott theory proved successful in calculations of electrical resistivity of vacancies in nickel [16]. The charge carrier concentration, necessary for these calculations, was evaluated from the values of an average magnetic moment μ. For Ni, which has $\mu = 0.54\mu_B$ and 10 $(s + d)$-electrons per atom, the carrier concentration in the *s*-band is $n_s = 0.54$ electrons per atom; the same number of holes is present in the *d*-band. In the case of Co, which has 9 $(s + d)$-electrons per atom and $\mu = 1.72\mu_B$, $n_s = 0.72$ electrons per atom. In these metals, according to the Hund rule, one of the *d*-subbands (↑) is completely occupied, and the other (↓) is partially free, it is natural to suppose [16] that the effective number of charge carriers in the *s*-band is $n_s^* = n_s/2$, because the spin down (↓) *s*-electrons scatter to the *d*-subband, and only the remaining spin up (↑) electrons from the *s*-band contribute to the scattering at defects. This is so for the metals situated at the end of the transition metals period, where $N_d(\varepsilon_F) \gg N_s(\varepsilon_F)$. However, for the metals from the beginning or the middle of the period (here these are Ti, Zr, Mo, and W) that have vacant states in both *d*-subbands, it is more appropriate to consider that the probability of *s*-electrons' scattering to the vacant states of the *s*- and *d*-bands is proportional to the electronic densities of states in these bands. Then, according to [17], we can write

$$\frac{1}{\tau_s} = \frac{1}{\tau_{sd}} + \frac{1}{\tau_{ss}},$$

where τ_s represent the relaxation times of the corresponding scattering processes. If we assume that the coupling constants are the same, then τ_{ss}^{-1} and τ_{sd}^{-1} become proportional to the densities of states N_s and N_d at the Fermi level. Therefore, the total concentration of *s*-electrons with spins up and down will be subdivided into two parts (i.e., $n_s = n_{sd} + n_{ss}$) in the proportion $n_{sd}/n_{ss} = N_d/N_s$. Thus, only n_{ss} electrons will contribute to the scattering by the lattice defects, that is, the effective number of charge carriers is $n_s^* = n_{ss}$.

The values of n_s and n_s^* for different metals, considered in the present study, are presented in Table 1 together with the structural data (the structure type and lattice parameters) and the group number in the Periodic Table. For metals such as Be, Zn, Cd, Al, Ti, Zr, Mo, W, and Pd the values of n_s were taken from the band structure calculations, reviewed and generalized in [7]. The effective charge carrier concentration n_s^* for Ti, Zr, Mo, and W was evaluated from the data on the electronic heat capacity coefficient, which is proportional to the electronic density of states at the Fermi level. According to the data, presented in [18], average values of γ for Ti, Zr, Mo, and W are respectively 8.1, 6.9, 5.0, and 2.6 in units of 10^{-4} cal mol^{-1} K^{-2}. Expressed in the units of the copper density of states (the γ_{Cu} value for copper is 1.66×10^{-4} cal mol^{-1} K^{-2} the densities of states N_{d+s} for these metals are 4.8, 4.1, 3.0, and 1.5, respectively. The density of states in the *s*-band of these metals with respect to corresponding quantity in copper can be evaluated using the free-electron model if we assume that $N_s(\varepsilon_F) \sim n_s^{1/3}$. In such a way the densities of states in the *s*-band of Ti, Zr, Mo, and W can be estimated as 0.40, 0.40, 0.76, and 0.62 (in the units of the copper density of states). From these data we calculated the values of $n_{ss} = n_s^*$, presented in Table 1.

The effective Fermi wave vector of conduction electrons was calculated similarly to [16] as

$$k_F^* = (3\pi^2 n_e)^{1/3}, \tag{1}$$

Table 1. Crystal structure, lattice parameters, and charge carrier concentration in metals under consideration

Metal	Group number	Structure	a, 10^{-10} m	c, 10^{-10} m	n_s, electron per atom	n_s^*, electron per atom
Cu	I*B*	fcc	3.61		1	1
Au	I*B*	fcc	4.08		1	1
Be	II*A*	hcp	2.29	3.58	0.032	0.032
Zn	II*B*	hcp	2.66	4.95	0.09	0.09
Cd	II*B*	hcp	2.98	5.62	0.095	0.095
Al	III*B*	fcc	4.05		1	1
Ti	IV*B*	hcp	2.95	4.69	0.065	0.0054
Zr	IV*B*	hcp	3.23	5.15	0.065	0.0064
Mo	VI*B*	bcc	3.15		0.44	0.112
W	VI*B*	bcc	3.16		0.24	0.097
Fe	VIII	bcc	2.87		0.22	0.11
Co	VIII	hcp	2.51	4.07	0.72	0.36
Ni	VIII	fcc	3.52		0.54	0.27
Pd	VIII	fce	3.89		0.55	0.275
Pt	VIII	fcc	3.92		0.42	0.21

where $n_e = n_s^* / \Omega$ is the effective charge carrier concentration per unit volume; Ω is the atomic volume (in what follows we will omit the sign * as a superscript to k_F).

CALCULATION OF ELECTRICAL RESISTIVITY OF DISLOCATIONS

Calculations of the scattering cross-section Q of conduction electrons by dislocations was carried out using the partial-waves technique. In our calculations we supposed that the main contribution to the scattering of electrons arises from the cores of dislocations, and we thus neglected the scattering by elastic fields of dislocations. The values of Q were calculated by solving the Schrödinger equation for the axially symmetric potential of the type

$$V(r) = \begin{cases} -V, \ r < R_1 \\ V_0, \ R_1 \le r \le R_2 \\ 0, \ r > R_2 . \end{cases} \tag{2}$$

The potential of this type allows accounting for the main features of lattice distortions in the region of dislocation core, namely, the lattice expansion region that contains an excess negative charge and the adjacent region of the lattice compression, the presence of which is the reason for formation of quasistationary states with small lifetimes $\tau \sim h / \Gamma$, where Γ is the width of the level. Potential of the same type was obtained in [19] for a screw dislocation, using the pseudoatomic model that takes into account the atomic displacements in the region of dislocation core and the deformation of elastic continuum of the surrounding matrix. Among the potentials, leading to quasistationary states in the positive energy range, the potential (2) is the simplest one. We assume that the external radius of the potential R_2 is equal to the atomic radius. For the internal radius we took $R_1 = R_2 / 2$. The latter choice is somewhat conditional, but it does not affect significantly the results. The potential well depth V was adjusted to make the position of the quasistationary level ε_r coincident with the Fermi energy ε_F

$$\varepsilon_r \approx \varepsilon_F = \frac{\hbar^2}{2m} k_F^2 . \tag{3}$$

This was done because only electrons with energy close to ε_F (within several thermal energies) contribute to the transport properties. The height of the potential barrier V_0 was chosen based on the screening condition for the defect charge by the cloud of rearranged conduction electrons.

Because of the cylindrical symmetry of the problem, we can represent the wave function in the form

$$\psi(r, z, \varphi) = e^{ik_z z} \sum_{n=-\infty}^{\infty} P_n(r) e^{in\varphi} . \tag{4}$$

Substituting this function in the Shrödinger equation, we obtain the equation for the radial function

$$P_n'' + \frac{1}{r} P_n' + \left[k_\perp^2 - \frac{2m}{\hbar^2} V - \frac{n^2}{r^2} \right] P_n = 0, \tag{5}$$

where $k_\perp = (k_F^2 - k_z^2)^{1/2}$ is the transverse component of the wave vector. Therefore, the problem reduces to the Bessel equation, the solutions to which are the Bessel functions with the arguments, $\kappa_0 r$, κr, and $k_\perp r$ in the regions $r < R_1$, $R_1 \le r \le R_2$, and $r > R_2$, respectively, where the quantities $\kappa = [k_\perp^2 + (2m / \hbar^2)V]^{1/2}$ and $\kappa_0 = [k_\perp^2 - (2m / \hbar)V_0]^{1/2}$. The phase shifts were calculated using the scattering matrix formalism. There are two linearly independent solutions of (5), $\varphi^-_{\mathbf{k}n}$ and $\varphi^+_{\mathbf{k}n}$, corresponding to the incident and scattering waves. It is known that if we construct the regular in zero function

$$\varphi^0_{\mathbf{k}n} = a_n(\mathbf{k}) \varphi^-_{\mathbf{k}n} + b_n(\mathbf{k}) \varphi^+_{\mathbf{k}n}, \tag{6}$$

the scattering matrix will take the form

$$S_n(\mathbf{k}) = \frac{b_n(\mathbf{k})}{a_n(\mathbf{k})}, \tag{7}$$

where $\mathbf{k} = k_1 + ik_2$ is the generalized wave vector.

As the most general solution to (5), we choose the function $\varphi^+_{\mathbf{k}n} = P^+_{\mathbf{k}n}(r)$ in the form

$$\varphi^+_{\mathbf{k}n} = \begin{cases} H_n^{(1)}(k_\perp r), \ r > R_2 \\ c_n I_n(\kappa_0 r) + d_n K_n(\kappa_0 r), \ R_1 \le r \le R_2 \\ g_n H_n^{(1)}(\kappa r) + f_n H_n^{(2)}(\kappa r), \ r < R_1 . \end{cases} \tag{8}$$

The solution $\varphi^-_{\mathbf{k}n}$ is obtained as a complex conjugate. The analysis of these solutions shows that the scattering matrix can be represented as

$$S_n(\mathbf{k}) = \frac{f_n^* - g_n^*}{g_n - f_n} . \tag{9}$$

Using this expression, we can determine the phase shifts accounting for the quasistationary states. It is known that these states correspond to the complex poles of $S_n(\mathbf{k})$ in the lower semiplane of the wave vector $\mathbf{k}$. Quasistationary levels are characterized by the resonance energy ε_0 and the width of the resonance Γ. These quantities are related to the components of the complex wave vector $k_1^0 + ik_2^0$, at which the scattering matrix has a pole, as follows

$$\begin{gathered} \varepsilon_0 = \frac{\hbar^2}{2m} [(k_1^0)^2 - (k_2^0)^2] ; \\ \Gamma = \frac{2\hbar^2}{m} k_1^0 k_2^0 . \end{gathered} \tag{10}$$

The most general expression for $S_n(\mathbf{k})$ with a pole determining the quasistationary level is

$$S_n(\mathbf{k}) = e^{i2\eta_n} = e^{i2\alpha_n}\frac{\varepsilon - \varepsilon_{0,n} - \dfrac{i\Gamma_n}{2}}{\varepsilon - \varepsilon_{0,n} + \dfrac{i\Gamma}{2}}, \tag{11}$$

where η_n and α_n are the total and potential scattering phases. For the total phase we obtain

$$\eta_n = \alpha_n - \operatorname{atan}\frac{\Gamma_n}{2(\varepsilon - \varepsilon_{0,n})} \equiv \alpha_n - \beta_n. \tag{12}$$

Here β_n is the resonance scattering phase. Far from the resonance the contribution of the resonance term to η_n decreases considerably, and the scattering matrix can be written as

$$S_n = e^{i2\alpha_n}. \tag{13}$$

Comparing (13) and (9), we obtain for the potential phase

$$\tan\alpha_n = \frac{\operatorname{Im}(f_n - g_n)}{\operatorname{Re}(g_n - f_n)}.$$

Using the condition of continuity of the wave function and of its first derivative at the points R_1 and R_2 we finally obtain

$$\tan\alpha_n = \frac{A_n}{B_n}, \tag{14}$$

where

$$\begin{aligned}A_n = \kappa k_\perp \{&J_n'(\kappa R_1) J_n'(k_\perp R_2)\,[I_n(\kappa_0 R_2) K_n(\kappa_0 R_1) - I_n(\kappa_0 R_1) K_n(\kappa_0 R_2)\,]\,\}\\ + \kappa\kappa_0 \{&J_n'(\kappa R_1) J_n(k_\perp R_2)\,[I_n(\kappa_0 R_1) K_n'(\kappa_0 R_2) - I_n'(\kappa_0 R_2) K_n(\kappa_0 R_1)\,]\,\}\\ + \kappa_0 k_\perp \{&J_n(\kappa R_1) J_n'(k_\perp R_2)\,[I_n'(\kappa_0 R_1) K_n(\kappa_0 R_2) - I_n(\kappa_0 R_2) K_n'(\kappa_0 R_1)\,]\,\}\\ + \kappa_0^2 \{&J_n(\kappa R_1) J_n(k_\perp R_2)\,[I_n'(\kappa_0 R_2) K_n'(\kappa_0 R_1) - I_n'(\kappa_0 R_1) K_n'(\kappa_0 R_2)\,]\,\},\end{aligned}$$

and B_n can be obtained by substituting the functions $N_n(k_\perp R_2)$ and $N_n'(k_\perp R_2)$ for $J_n(k_\perp R_2)$ and $J_n'(k_\perp R_2)$, respectively.

To calculate the resonance levels, one has to find the poles of the scattering matrix, that is, the roots of the equation $c_n = d_n$; the complex nature of these roots should be taken into account. The solution of the problem leads to the equation

$$\begin{aligned}&\kappa k_\perp H^{(1)}_{n+1}(k_\perp R_2) J_{n+1}(\kappa R_1)\,[I_n(\kappa_0 R_2) K_n(\kappa_0 R_1) - I_n(\kappa_0 R_1) K_n(\kappa_0 R_2)\,]\\ &+ \kappa\kappa_0 H^{(1)}_{n+1}(k_\perp R_2) J_{n+1}(\kappa R_1)\,[I_n(\kappa_0 R_1) K_{n+1}(\kappa_0 R_2) + I_{n+1}(\kappa_0 R_2) K_n(\kappa_0 R_1)\,]\\ &= \kappa_0 k_\perp H^{(1)}_{n+1}(k_\perp R_2) J_n(\kappa R_1)\,[I_{n+1}(\kappa_0 R_1) K_n(\kappa_0 R_2) + I_n(\kappa_0 R_2) K_{n+1}(\kappa_0 R_1)\,]\\ &+ \kappa^2 H^{(1)}_n(k_\perp R_2) J_n(\kappa R_1)\,[I_{n+1}(\kappa_0 R_1) K_{n+1}(\kappa_0 R_2) - I_{n+1}(\kappa_0 R_2) K_{n+1}(\kappa_0 R_1)\,].\end{aligned} \tag{15}$$

Solving this equation, we determine the parameters of the resonance level $\varepsilon_{0,n}$ and Γ_n, as well as the resonance phase shift β_n.

The transport scattering cross section Q, averaged over the angle φ, is expressed through the phase shifts as follows:

$$Q = \frac{8}{\pi k_F}\int_0^{\pi/2}\sum_{n=0}^{\infty}\sin^2(\eta_n - \eta_{n+1})\,d\varphi. \tag{16}$$

Within the relaxation time approximation, the change in electrical resistivity per unit dislocation density is

$$\frac{\rho_d}{N_d} = \frac{m^* v_F Q}{n_e e^2} = \frac{\hbar k_F \Omega Q}{n_s^* e^2}, \tag{17}$$

where m^* is the effective mass of charge carriers equal to $\hbar k_F / v_F$.

The height of the potential barrier V_0 was determined from the screening condition, which for linear defects has the form [4]

$$\xi = \frac{2k_F}{\pi^2}\int_0^{\pi/2}\sum_{n=-\infty}\eta_n(\varphi)\sin\varphi\,d\varphi, \tag{18}$$

where ξ is the linear charge density along the dislocation line, expressed in units of electron charge. According to [20], the lattice dilatation in the region of dislocation core, calculated per unit dislocation length, lies in the range $dV = b_B^2$ - $4b_B^2$. In the present work we assume that $dV = b_B^2$ and, therefore, ξ is determined as $\xi = dV/\Omega$. Only the stable Burgers vectors b_B of perfect dislocations in corresponding crystal structures were considered, i.e., we have chosen b_B equal to $1/2\langle 110\rangle$ or $a\sqrt{2}/2$ for fcc metals; $1/2\langle 111\rangle$ and $\langle 100\rangle$ or $a\sqrt{3}/2$ and a for bcc metals; and $1/3\langle 11\bar{2}0\rangle$ and $\langle 0001\rangle$ or a and c for hcp metals (a and c are the lattice parameters). Table 2 presents the results of the calculations of ρ_d / N_d. Two values, given for some metals, correspond to the smaller and larger Burgers vectors. For the smaller b_B we also present the potential parameters V and V_0 and the width of the resonance level Γ. For comparison we include in Table 2 the results of calculations of other works, as well as the experimental data avail-

Table 2. Parameters of scattering potential and resistivity of the unit density of dislocations

Metal	V, 10^{-19} J	V_0, 10^{-19} J	Γ, 10^{-19} J	ρ_d / N_d, 10^{-13} $\mu\Omega$ cm^3				
				This work	Previous calculations [7]	Previous calculations [13]	Experimental data	
Cu	28.2	15.0	4.1	1.7	1.3	0.78	1.6 ± 0.2*	2.3 [23]
Au	22.0	11.7	3.3	2.4	1.9	1.2	2.6	1.9 [25]
Be	47.9	39.3	0.9	7.3 - 18.2	28.0	22.0	34.0	3.0 - 25.0**
Zn	23.7	22.3	1.3	5.5 - 26.9				
Cd	18.7	17.6	1.1	7.7 - 36.3	25.0	7.3	24	5**
Al	22.9	12.2	3.1	2.5	1.8	1.0	1.7 ± 0.3	3.2 [23]
Ti	22.9	21.1	1.0	94.3 - 370.4	29		100	
Zr	19.4	17.7	0.8	101.7 - 371.6	40	15	100	40**
Mo	19.8	16.0	3.1	9.8 - 16.0	3.7	3.8	5.8	22 [24]
W	20.6	18.7	2.3	7.7 - 12.5	7.4	12.5	7.5	19 [25]
Fe	24.4	22.7	2.8	4.7 - 8.1	1.9	9.1	10 ± 4	7 ± 3**
Co	27.5	17.9	4.1	3.4 - 10.0				
Ni	27.2	20.0	3.7	3.8	1.1	3.0	10	2.8 ± 0.5**
Pd	22.1	16.2	3.1	5.1				
Pt	21.4	17.2	2.8	5.6	4.0	2.5	9	3.5**

*Note: * cited in Ref. [7].*
*** cited in Ref. [13].*

able in the literature. In our calculations we satisfy the screening condition (18) within an accuracy of 10^{-2} and take into account six ($n = 6$) phases.

CALCULATION OF ELECTRICAL RESISTIVITY OF GRAIN BOUNDARIES

Presently, it is beyond question that the low-angle grain boundary (that is, the boundary with the misorientation angle θ up to 10 - 15°) consists of separate dislocations. In the symmetrical tilt boundaries of cubic lattices the spacing between dislocations is

$$D^l = \frac{b_B}{2\sin(\theta/2)} \approx \frac{b_B}{\theta}. \qquad (19)$$

An asymmetric low-angle grain boundary that has both tilt and twist components can generally be described by three independent sets of dislocations with noncoplanar Burgers vectors. We consider, for simplicity, only the symmetric tilt boundaries with misorientation axes along the directions $\langle 100 \rangle$ for fcc, $\langle 110 \rangle$ for bcc and $\langle 0001 \rangle$ for hcp structures. As shown in [14], the change in electrical resistivity per unit density of a low-angle grain boundary is

$$\frac{\rho_G^l}{N_G} = \frac{\rho_d}{N_d D^l}. \qquad (20)$$

There are a great number of models for high-angle grain boundaries. These are the model of amorphous layer, the model of islands, the model of liquid boundary, the model of partial dislocations, the disclination model, etc. Reference [21] reviews these models. These models share one common feature that differentiates them from the models of low-angle grain boundaries. This feature is the considerably higher looseness, or porosity, of the high-angle grain boundary. Atomistic calculations of stable configurations clearly show that cylindrical pores are present inside the high-angle grain boundaries [22]. For this reason, in the present work we approximated the high-angle grain boundary ($15° \le \theta \le 45°$) by a set of cylindrical pores. According to [2], the spacing between the pores in cubic lattices is given by $D^h = a / 2\sin(\theta/2)$.

In hcp crystals we considered the tilt boundaries in the $\{11\bar{2}0\}$ planes, formed by linear defects parallel to the $\langle 0001 \rangle$ direction. Taking into account that in hcp crystals gliding proceeds along the most closely packed planes $\{0001\}$, we assumed the spacing D between linear defects in both low- and high-angle boundaries to be

$$D = \frac{a\sin(60° - \theta/2)}{2\sin(\theta/2)}. \qquad (21)$$

The electrical resistivity of high-angle grain boundaries was calculated as

$$\frac{\rho_G^h}{N_G} = \frac{\rho_p}{N_p D^h}, \qquad (22)$$

where ρ_p / N_p is the electrical resistivity of cylindrical pores evaluated using (17) with the scattering cross section Q given by (16). The phase shifts η_n, entering into (16), were calculated using the axially symmetrical potential of the type

Table 3. An increase of electrical resistivity per unit density of cylindrical pores and grain boundaries, averaged in corresponding ranges of misorientation angles

Metal	ρ_p / N_p, 10^{-13} $\mu\Omega$ cm^3	ρ_G^l / N_G, 10^{-12} Ω cm^2	ρ_G^h / N_G, 10^{-12} Ω cm^2	ρ_G / N_G, 10^{-12} Ω cm^2		
				This work	Previous calculations [11]	Experimental data
Cu	2.4	0.9	4.0	2.9	2.2	1.8 - 3.1*
Au	3.4	1.1	5.0	3.7	2.8	3.5*
Be	3.5 - 14.9	5.0 - 12.5	8.0 - 33.7	6.5 - 23.1		
Zn	5.7 - 28.5	3.3 - 16.0	11.0 - 55.4	7.1 - 35.7	27.1	4.0 - 55.0 [26]
Cd	7.9 - 40.0	4.1 - 19.2	13.8 - 69.5	8.9 - 44.4	32.6	15.0 - 19.1 [26]
Al	3.4	1.1	5.0	3.7	2.7	1.1 - 2.4*
Ti	94.7 - 354	50.5 - 198	166 - 623	108 - 410		
Zr	104 - 399	49.8 - 179	166 - 640	108 - 409		
Mo	9.9 - 12.0	4.7 - 6.7	18.9 - 22.9	14.2 - 17.5	18.0	8.8*
W	7.2 - 8.9	3.7 - 5.2	13.7 - 16.4	10.4 - 12.6	22.0	20*
Fe	4.6 - 5.6	2.5 - 3.7	9.6 - 11.7	7.2 - 9.1	6.2	80 - 160*
Co	4.7 - 10.3	2.2 - 6.3	9.6 - 21.3	5.9 - 13.8	2.4	5.0*
Ni	5.9	2.0	10.1	7.4	1.9	5.0 - 14.0*
Pd	7.9	2.4	12.2	8.9		
Pt	9.0	2.7	13.7	10.1		

*Note: * cited in Ref. [13].*

$$V(r) = \begin{cases} V_0, r \le R_2 \\ 0, r > R_2. \end{cases} \quad (23)$$

For this potential, the expression for η_n was obtained in [14]. The linear charge density ξ was assumed to be the same as for dislocations.

The range of misorientation angles from 10 to 25° was treated as a transient one, that is, we supposed that the grain boundaries with such misorientations consisted of both dislocations and cylindrical pores. With increasing θ the fraction of dislocations x decreases and the fraction of pores $(1 - x)$ increases. The electrical resistivity of grain boundaries ρ_G / N_G in this range of misorientation angles was calculated as

$$\frac{\rho_G}{N_G} = \frac{x\rho_d}{D^l N_d} + \frac{(1-x)\,\rho_p}{D^h N_p}. \quad (24)$$

From the crystal symmetry considerations it follows that the misorientation of the lattice with respect to directions considered here has the periodicity $\pi/2$ for the cubic structures and $\pi/3$ for the hcp structure. Therefore, the maximum misorientation is 0 = 45° for the bcc and fcc metals and $\theta = 30°$ for the hcp metals.

The calculated grain boundary contributions to electrical resistivity ρ_G / N_G, averaged over misorientation angles of 0 to 45° for the cubic metals and 0 to 30° for the hcp metals, are presented in Table 3. Also presented are the values of electrical resistivity of cylindrical pores per their unit concentration ρ_p / N_p, and the mean values of electrical resistivity of low-angle and high-angle grain boundaries, averaged over the corresponding angular intervals. The results of [11] on calculations of ρ_G / N_G and available experimental data are also included for comparison. The mean distances between linear defects in low-angle and high-angle ranges were assumed to be $\overline{D}^l_{\text{fcc}} = 5.4a$, $\overline{D}^h_{\text{fcc}} = 1.7a$, $\overline{D}^l_{\text{bcc}} = 6.6a$, $\overline{D}^h_{\text{bcc}} = 1.7a$, and $\overline{D}_{\text{hcp}} = 3.0a$.

CONCLUSION

We calculated the values of electrical resistivity of dislocations and grain boundaries in polyvalent and transition metals, using the model that takes into account the lattice dilatation in the region of dislocation core and the presence of quasistationary states. Based on the data presented in Tables 2 and 3, we may conclude that the calculated results agree fairly well with the available experimental data. In most cases the agreement with experimental data is better than in earlier calculations.

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